Small Business Innovation Research/Small Business Tech Transfer

# Compact Kinetic Mechanisms for Petroleum-Derived and Alternative Aviation Fuels, Phase II



Completed Technology Project (2015 - 2018)

## **Project Introduction**

To be useful for computational combustor design and analysis using tools like the National Combustion Code (NCC), low-dimensional chemical kinetic mechanisms for modeling of real fuel combustion chemistry must be sufficiently compact so that they can be utilized in multi-dimensional, multiphysics, reacting computational fluid dynamics (CFD) simulations. Despite advances in CFD-appropriate kinetic mechanism reduction for kerosene-range fuels, significant combustion property variation among current and prospective certified fuels remains a challenge for meaningful CFD-advised design of high pressure, low-emissions combustors. The proposed project will leverage Princeton's ongoing work in aviation fuel surrogate formulation and modeling as well as kinetic mechanism development for emissions and high pressure combustion to produce and demonstrate a meta-model framework for automated generation of fuel-flexible compact chemical kinetic mechanisms appropriate for 3-D combustion CFD codes. During Phase I, Compact Mechanisms for both an alternative, natural-gas derived synthetic kerosene and a conventional petro-derived Jet A kerosene have been developed and demonstrated. Results indicated that, over a very broad range of pressures, temperatures, equivalence ratios, and characteristic times, these Compact Mechanisms well reproduce predictions of global combustion behaviors (ignition, extinction, heat release rate, pollutant mole fractions) relative to predictions of significantly larger target chemical kinetic mechanisms. Technical objectives for Phase II R&D include development of a stand-alone software application for generation of tailor-made, fuel-specific Compact Mechanisms, and demonstration of Compact Mechanism performance in computation-intensive CFD applications. Achievement of these objectives together will advance the current state of this R&D program to TRL 5.



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## **Primary U.S. Work Locations and Key Partners**



Organizations Performing Work	Role	Туре	Location
Spectral Energies, LLC	Lead Organization	Industry Small Disadvantaged Business (SDB)	Dayton, Ohio
Glenn Research Center(GRC)	Supporting Organization	NASA Center	Cleveland, Ohio

## **Primary U.S. Work Locations**

Ohio

## **Project Transitions**

O

May 2015: Project Start



October 2018: Closed out

### **Closeout Documentation:**

• Final Summary Chart(https://techport.nasa.gov/file/137749)

# Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

**Lead Organization:** 

Spectral Energies, LLC

**Responsible Program:** 

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## **Project Management**

**Program Director:** 

Jason L Kessler

**Program Manager:** 

Carlos Torrez

**Principal Investigator:** 

Sivaram P Gogineni

**Co-Investigator:** 

Sivaram Gogineni



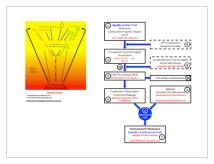
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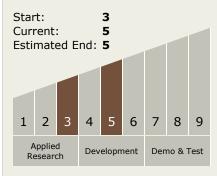
## **Images**



## **Briefing Chart**

Compact Kinetic Mechanisms for Petroleum-Derived and Alternative Aviation Fuels Briefing Chart (https://techport.nasa.gov/imag e/127690)





## **Technology Areas**

### **Primary:**

## **Target Destinations**

The Sun, Earth, The Moon, Mars, Others Inside the Solar System, Outside the Solar System

